

Performance of direct air capture process in honeycomb channel configuration: A CFD study

Majid Nejadseifi*. Shervin Karimkashi**. Tero Tynjälä*. Payman Jalali*

*Laboratory of Thermodynamics, School of Energy Systems, Lappeenranta-Lahti University of Technology, Lappeenranta, 53850, Finland (Tel: 358-415750813; e-mail: majid.nejadseifi@lut.fi, tero.tynjala@lut.fi, payman.jalali@lut.fi).

**Laboratory of Energy conversion and systems, Department of Mechanical Engineering, School of Engineering Sciences, Aalto university, Espoo, 02150, Finland (Tel: +358505602614; e-mail: shervin.karimkashiarani@aalto.fi)

Abstract: This study presents a kinetic reaction modeling method for direct air capture (DAC) process of CO₂ adsorption using computational fluid dynamics (CFD). Here, CO₂ is adsorbed by amine coated air-surface contact area. The Langmuir model is employed to represent the kinetics of CO₂ adsorption. Despite neglecting the diffusive phase of the adsorption, which is dominant only in the later stages of adsorption, the surface reaction model gives a satisfactory representation of the adsorption for a major part of the process. Honeycomb reactors with coated adsorbent may yield a better control of reaction rate and pressure drop compared to commonly used packed bed adsorption columns. Their enhanced performance in distributing the flow homogeneously between and within channels creates unique features for the reactor. In this study, we have analyzed mechanical and electrical energy demand for adsorbing CO₂ per unit mass of adsorbed CO₂ as a function of air flow rate. Adsorption performance of honeycomb structure is anticipated to significantly improve in comparison to the packed beds.

Keywords: CFD, Hexagonal channel, adsorption, Direct Air Capture, surface reaction

1. INTRODUCTION

From scientific viewpoints, excess amount of CO₂ in atmosphere causes climate change with making oceans more acidic (Wang et al., 2011). As the solution for this problem, we need to replace fossil primary energy sources with CO₂ neutral energy sources. However, there is still a significant release of CO₂ (33 billion tons per year in 2021) which indicates great challenges ahead of fixing global warming (Zhongming et al., 2021). The negative consequences of CO₂ accumulation in the atmosphere will exist for thousands of years, even if emissions stop today (Solomon et al., 2009). So, there will be also needed to remove CO₂ out of the atmospheric air, which is addressed as negative emissions. In this context, we should increase annual CO₂ removals from the atmosphere to 10 billion tons of CO₂ by 2050 (McQueen et al., 2021). It is a challenging objective, which makes scientists to explore different ways to find the most efficient method. One promising method is the Direct Air Capture (DAC), which removes CO₂ directly from the air (Sanz-Pérez et al., 2016).

In order to obtain a comprehensive and detailed analysis, computational fluid dynamics (CFD) simulations can be performed. In a series of studies (Deutschmann et al., 2001; Tischer and Deutschmann, 2005; Nejadseifi et al., 2024), a modern multi-dimensional approach to detailed modeling of fluid flow transfer processes and chemical kinetics have been developed. Specifically, there has been critical evaluation of plug flow, boundary layer, and general three-dimensional models for simulating steady-state transport processes and chemistry in a honeycomb channel flow (Klenov et al., 2009).

In any gas-solid contact system, such as in CO₂ capture processes, maximizing the interface between gas and solid surfaces while minimizing the pressure drop is a crucial goal. This enhances CO₂ capture efficiency and reduces the energy required for blowing air in direct air capture (DAC) systems. Ceramic monoliths, due to their high surface area to volume ratio, have emerged as prime candidates for DAC contactors. They serve as excellent supports for CO₂ sorbents, as demonstrated by several studies (Choi et al., 2011; Rodriguez-Mosqueda et al., 2018; Thakkar et al., 2016). Monoliths are also recognized for their minimal pressure drop (Thakkar et al., 2016). Recently, Fu and Davis (2023) demonstrated that employing monoliths as air contactors in DAC significantly reduces energy consumption compared to fixed beds. Verougstraete et al. (2020) have proposed the use of a carbon monolith for DAC to facilitate rapid heating and cooling, thereby achieving shorter adsorption-desorption cycles. Monoliths are comprised of straight channels with various cross-section shapes. Depending on their intended application, monoliths can adopt cylindrical, cubic, or hexagonal shapes. Sorbents are applied to the walls of these channels. In the case of CO₂ capture, gaseous CO₂ diffuses from the air stream to the walls of the monolith channels, where it is subsequently adsorbed by the sorbents. Improving the transfer of CO₂ to the sorbent surface means a higher process efficiency and energy saving (Jiang et al., 2023).

In this paper, simulations are carried out for monolithic contactor reactor with conventional straight channels. By changing the hexagonal channel flow rate, we promote the CO₂ transport to the sorbent-gas interface and investigate its

effect on CO₂ capture rate. Simulations are conducted under atmospheric pressure and isothermal conditions at 25 C. The computational CFD package of ANSYS-Fluent, V. 2021 R2 has been used for the simulations. Upon solving the governing equations, steady flow profiles across the channel, local mass conversion between channel surface and gas, variation of CO₂ concentration at the channel outlet, pressure drop across the channel and power consumption per absorbed CO₂ are investigated.

2. METHODOLOGY

2.1 Sorbent coating and reactor model

In our simulations, a solid sorbent coat on an aluminum support of hexagonal straight channels is constructed. Typical samples of such hexagonal monoliths are presented in Fig. 1 and cross section of meshed symmetrical view in Fig. 2. For simplifying simulations, one sixth of the hexagonal cross section is considered (triangular symmetrical channel). The schematic of the single symmetrical hexagonal reactor is shown Fig. 1, where the air flows through. Considering narrow channel and lower flow velocities, the air flow can be assumed confidently laminar.

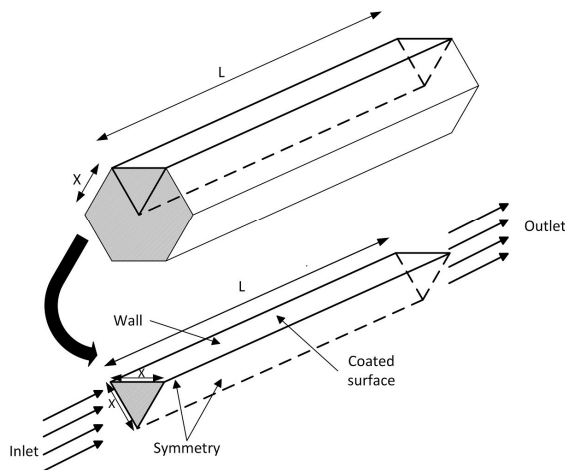


Fig. 1. A. schematical view of the symmetric hexagonal channel.

2.2 Mathematical description of Transport Equations:

The steady flow and transient reactive flow of air including CO₂ is simulated in the hexagonal channel in which CO₂ reacts with the sorbent covering the walls of the hexagonal channel. First, steady flow is solved and only the reaction part is transient. Due to small amount of CO₂ in the air flow, it is assumed that the reactions don't have any effect on flow. The Navier–Stokes equations(1,2,3) for incompressible single-phase fluid (air) solved. Mass transport equation (1) considered as time dependent, but momentum equation (2), which is taken as steady state are:

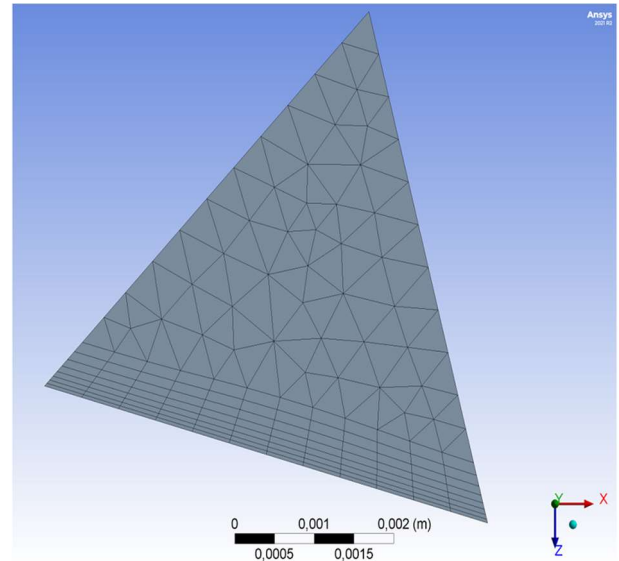


Fig. 2. Cross section mesh view of hexagonal channel cross section prepared for simulations.

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

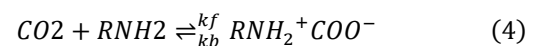
$$(\nabla \cdot \mathbf{u})\mathbf{u} = -\frac{\nabla p}{\rho} + \frac{\mu}{\rho} \nabla^2 \mathbf{u} \quad (2)$$

The inlet and outlet boundary conditions are velocity inlet and pressure outlet, respectively. No-slip wall boundary condition is applied over the sidewalls of the hexagonal channel. Flow is considered isothermal and energy equation is not taken into account, due to neglective share of adsorption heat to overall heat capacity of the flow. After solving steady Navier-Stokes equations for the velocity field, \mathbf{u} , it is used in the transient CO₂ species transport equation to solve it for CO₂ concentration C :

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = D \nabla^2 C \quad (3)$$

Here, C represents the concentration of CO₂ in the interstitial space, and D is the diffusion coefficient of CO₂ in air. There is no source term in this equation since CO₂ is not produced or consumed within the flow. However, CO₂ adsorption occurs over the reactive surface of the channel. We apply a surface reaction model over the surface to consider CO₂ adsorption. At the inlet, C is known and remains constant over time. The outlet is governed by a zero diffusive flux condition for CO₂. No mass flux is allowed through the sidewall except that made via reaction model.

For reaction, only simple one-step reaction is considered. The reaction rate is calculated at the wall surface for the reaction of CO₂ with amine. The following kinetic equations (4, 5) are taken as representative of several complex reactions:



$$r = k_{\text{langmuir}} C_{\text{CO}_2} \quad (5)$$

Equation (4) is the simplified representation of reactions, where capture of CO₂ occurs in the case of one primary amine group reacting with CO₂. (Choi et al., 2009; Elfving and Sainio, 2021; Sanz-Pérez et al., 2016). In (4) R is the chain of atoms which is not participating in the reaction. In real physics, there is both forward and backward reactions, however, the model assumes that reaction occurs only in forward direction. Note that at moderate temperature of 25°C, assuming the irreversibility of the adsorption process is plausible if the sorbent has a strong affinity for CO₂. Sorbent material properties used were same as in the adsorption modelling. Gas mixture inside the DAC-unit is estimated to contain only carbon dioxide (Elfving and Sainio, 2021). Equation (5) shows the relation between reaction rate r and concentration of reaction mixture components CO₂ (C_{CO_2}). Also, r is the reaction rate based on Langmuir kinetic model and $k_{langmuir}$ is the reaction kinetic constant. The Langmuir equation assumes that the adsorption of the gas to the sorbent is a reversible process and occurs only on a homogeneous surface with a fixed number of adsorption sites without considering the effects of the water vapor (one-step process). Since the purpose is to focus mainly on the adsorption of CO₂ during fast adsorption phase, selected single-step process model is considered to be sufficient for the analysis. Reaction kinetic constant $k_{langmuir}$ is obtained from fitting simulation results to the experiments (Elfving and Sainio, 2021). The fitting results are specific to a given reaction and depend on temperature, humidity, and other reaction conditions. The unit of k depends on the order of the reaction, which can be determined experimentally. For the case of CO₂ adsorption, the rate of reaction is directly proportional to the concentrations of both CO₂ and the adsorbent. This means that increasing the concentration of sorbent or CO₂ will increase the rate of reaction.

3. RESULTS AND DISCUSSION

3.1 Fluid flow, pressure drop, concentration.

The calculation of pressure drop is performed in various mesh sizes to verify the mesh independence. As seen from Fig. 2, we have used 12 meshes per reactive side of the hexagon(wall). In near wall, there is boundary layer and also surface reaction occurrence; therefore, it's necessary that meshes near wall is in layered shape and structured (hexahedral), while in the other regions only unstructured tetrahedral bigger meshes are enough. Table 1 shows the dependence of pressure drop on mesh resolution. For the coarse, fine and finer meshes, the number of nodes are 136421, 431597, 647372, respectively. The results for the pressure drop for different mesh sizes are shown in Table 1, which reveal the discrepancy in the pressure drop. The case with 12 mesh has the minimum difference with the neighboring number of meshes, and it can be chosen sufficient for the simulation. Flow is solved at steady state with 5000 iterations to ensure the convergence while the species transport model is off.

Six different inlet velocities, 0.004 m/s, 0.007 m/s, 0.01 m/s, 0.02 m/s, 0.1 m/s, 0.3 m/s are set for fixed hexagonal channel. The dependence of pressure drop-velocity is shown in Fig 3.

The results demonstrate a monotonic increase of pressure drop with velocity. Higher pressure drops mean a higher fan power requirement. In this work, length is kept constant although downsizing (shortening the channel length) can help with reducing the pressure drop.

Table 1. Mesh independence study.

Mesh per hexagon side(X)	Number of Nodes	Pressure drops per length (Pa/m)
8	136421(coarse)	0.5289
12	431597(fine)	0.5309
15	647372(finest)	0.5316

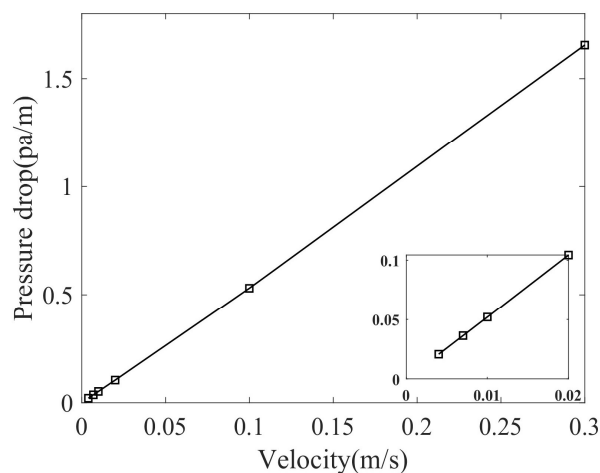


Fig. 3. Variation of pressure drop per unit length (Pa/m) with velocity(m/s). Hexagonal channel is 1 m. Air flow temperature is 25 °C and humidity is 2 %.

To understand the adsorption phenomenon inside hexagonal channel and its efficiency, it is essential to compare the results with other geometries. In previous works, adsorption performance of honeycomb structure is compared to the packed beds for different sorbents and gases and also for CO₂ adsorption. (Jänchen et al., 2015; Querejeta et al., 2022; Sakwa-Novak et al., 2016; Wajima et al., 2011). To this end, a simulation has been conducted also for the cylindrical packed bed system by the length of 1.77 cm and the diameter of 0.9 cm. This packed bed is consisted of particles with the diameter of 0.6 mm and particle volume fraction of 0.61. The working fluid temperature and humidity are taken as 25°C and 2%. The hexagonal channel length is 1.77cm, but its side length is allowed to have different values. Figure 4 represents the time variation of CO₂ concentration at the outlets of hexagonal unit and the packed bed during the adsorption process for the inlet velocity being as 0.13 m/s. Note that CO₂ adsorption on an

amine-based sorbent is fast. A key benefit of using hexagonal channels in a DAC contactor is the lower pressure drop, in comparison to the packed beds or the channels with other shapes of cross sections, while keeping the reactive area still high. Surface reactions serve as the main transport mechanism at this study. For qualitative comparison between hexagonal channels and packed beds, several hexagonal channels with various side lengths are considered in this study. Variation of the side length of hexagons affects the rate of adsorption and as seen in Fig. 4, for hexagon side $X=1.1$ mm, the results for hexagonal channel and packed bed channel are pretty close. In future works, we will optimize the channel based on geometry and compare the system with similar-capacity packed bed systems. Figure 4 indicates that in an adsorption system whether open channels like the hexagonal one or a packed bed, the sorbent saturates after some time. For instance, for the hexagonal channel with hexagon side of $X=1.1$ mm, as time advances to around 5000 seconds, the adsorption site starts to saturate which is similar to what happens in our studied packed bed (Nejadseifi et al., under preparation). Following this comparative study, we will demonstrate a wider study on hexagonal units having the length of 1 m, where we investigate the effects of velocity on adsorption process of CO₂. The purpose is to investigate the performance of hexagonal reactor for various flow rates. At some point, since there is no experimental data for hexagonal cases, but for the packed bed with small size (length =1.77 cm) experiments results were available and CFD simulation for packed bed fitted to them, while deviation was below 5% (Nejadseifi et al., under preparation; Elfving and Sainio, 2021). Therefore, for small scale hexagon with length of $L=1.77$ cm, result of CFD simulations qualitatively compared with packed bed. And at the following, we have used the same reaction coefficients for big size hexagonal channel.

Figure 5 shows the CO₂ outlet concentration variation with time for large hexagonal channels with the length of 1 m for the hexagonal side of 0.58 cm at different velocities. As it is observed, increasing the velocity shortens the time to reach saturation. For the velocity of $V=0.1$ m/s, the outlet CO₂ concentration begins to rise between the time 0.5×10^4 and

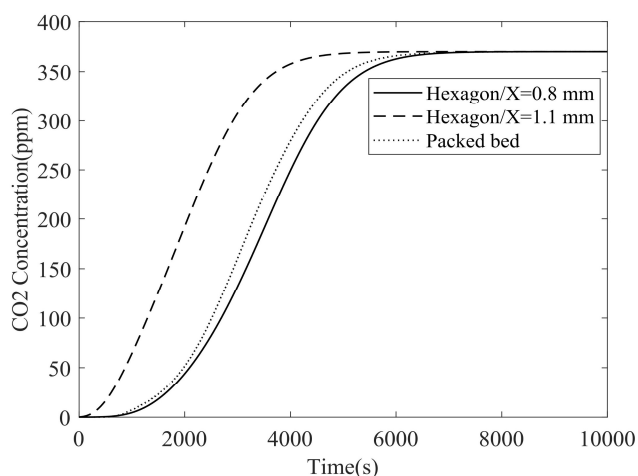


Fig. 4. CO₂ Concentration(ppm) variation at the outlet of hexagonal channel by time. Hexagonal channel and packed bed length is 1.77 cm. Air flow temperature is 25 °C and humidity is 2 vol-%. Velocity=0.13m/s.

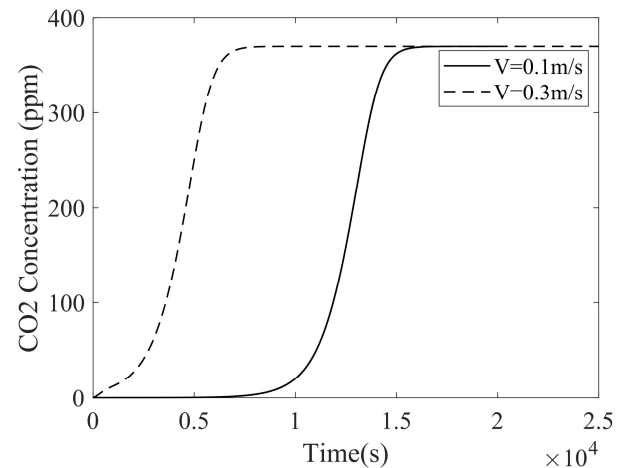


Fig. 5. CO₂ Concentration(ppm) change at the outlet of hexagonal channel by time. Hexagonal channel length is 1 m. Air flow temperature is 25 °C and humidity is 2 vol-%.

1.0×10^4 s. This is the time where system moves toward full saturation which is achieved around $\sim 1.0 \times 10^4$ s. For $V=0.3$ m/s, the outlet concentration rises almost from the beginning of the adsorption until it reaches full saturation around $t \sim 0.5 \times 10^4$ s.

3.2 Techno-economics of CO₂ capture in hexagonal channel

In designing a DAC system comprised of adsorption-desorption cycle in a monolithic contactor, air flow rate, as well as adsorption and desorption CO₂ concentration cut-off values (target CO₂ capture) play prominent roles in the final CO₂ capture cost. It should be mentioned that the focus of the current work is only on the adsorption stage. As the flow rate increases, more CO₂ is captured. However, higher flow rates are also associated with larger pressure drops that impose higher cost for consumed blowing power. Figures 6-8 present capture rates, demanded blowing (fan) power, and electricity consumption per ton of captured CO₂ for hexagonal channel contactor per unit length of channel at the side length of the hexagon as 0.58 cm. Air velocity ranges from 0.004 m/s to 0.3 m/s.

Figure 6 shows the variation of adsorption completion time (time for outlet concentration to reach 300 ppm) for a range of velocities between 0.004 and 0.3 m/s. Smaller panel inside Figs. 6-8 showed detailed values within small ranges of velocities. As it can be seen, increasing the velocity of air decreases the time of adsorption. However, experimental validations are required to confirm the performance of CO₂ adsorption at higher velocities.

In this study, the sensitivity analysis is aimed to obtain how the energy consumption related to air blow varies with air velocity as part of adsorption process, where the desorption stage is not considered. It can be noticed that in very small velocities, the saturation time increases exponentially as velocity decreases. Normally, very large saturation time

characterizes the adsorption process of DAC as inefficient or expensive from the energy consumption point of view.

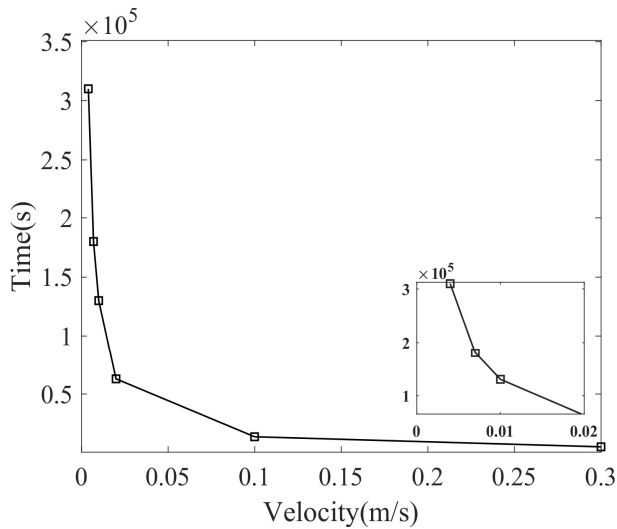


Fig. 6. Variation of adsorption reaction time (Time to reach 300 ppm) by velocity. Hexagonal channel length is 1 m. Air flow temperature is 25 °C and humidity is 2 vol-%.

The consumed blowing power cost per ton of captured CO₂ is estimated based on the assumption that the cost is proportional to the energy required in adsorption process. Based on the design of our DAC system, we assume that the energy is all provided by electricity. In the adsorption cycle, air is blown through the contactor and the contactor is kept at constant temperature (~25 °C). The blowing (fan) power for adsorption

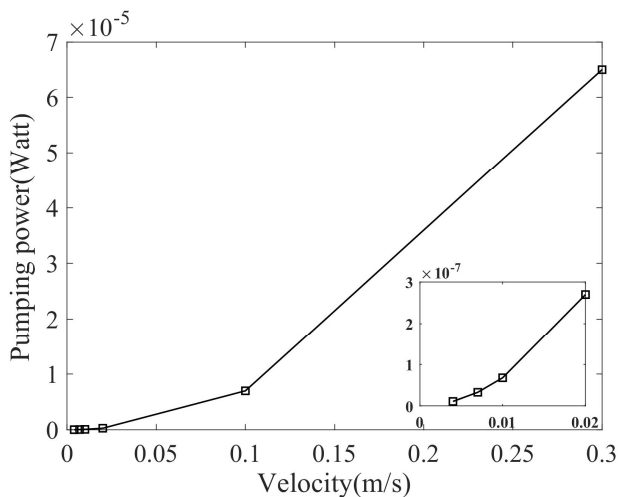


Fig. 7. Consumed blowing (fan) power vs. velocity. Hexagonal channel length is 1 m. Air flow temperature is 25 °C and humidity is 2 vol-%.

is therefore estimated by (6):

$$P = \frac{Q \cdot \Delta p}{\eta} \quad (6)$$

where P is the electrical power consumption during each adsorption cycle, ΔP is the air pressure drop for each hexagon, and Q is the volumetric flow rate of the air. The efficiency η is

the effectiveness of the system in converting electrical energy into mechanical energy to move the air, which is considered as a fixed value of 0.8. Figure 7 shows the variation of consumed power by velocity. For both higher ranges of velocities $0.1 \leq V \leq 0.3$ m/s and lower ranges $0.004 \leq V \leq 0.02$ m/s, we see a non-linear relation between the blower (fan) power and Velocity. Then, the total electricity consumption per ton of adsorbed CO₂ per each cycle is calculated by (7):

$$E = \frac{P \cdot t}{1000 \cdot m_{CO_2}} \quad (7)$$

where P is the electrical power consumption, t is the adsorption time of each cycle (the time for CO₂ concentration to reach 300 ppm). Obviously, it is not efficient to run the system after saturation. Also, m_{CO_2} is the amount of CO₂ adsorbed during each cycle. Figure 8 shows the electricity consumption per unit mass of CO₂ for various velocities, which displays the same trend as in Fig. 7 except for the lower range of velocity that turns to be linear.

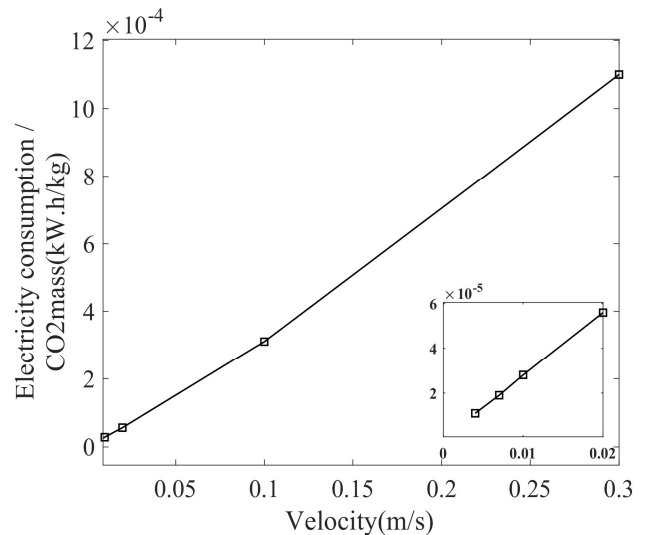


Fig. 8. Electricity consumption per / Adsorbed mass of CO₂.vs. velocity. Hexagonal channel length is 1 m. Air flow temperature is 25 °C and humidity is 2 vol-%.

4. CONCLUSIONS

Recently, CO₂ removal from air, also known as the Direct Air Capture (DAC), has attracted more attention due to its promise in reducing the greenhouse gas (GHG) emissions. However, costs associated with DAC have been the main obstacle for large-scale commercialization. Here, we presented a novel hexagonal shaped contactor and investigated performance of adsorption under various flow rates. Direct air flow inside straight channel is more commercialized with a higher demand because of its lower pressure drop, which makes it practical for large scale applications. Such a straight channel application is supposed to be more economic than non-straight channels or packed bed reactors. The techno-economic analysis showed how the adsorption stage is dependent of various air velocities. Focus of this work was on lower ranges of velocities ($V \leq 0.3$

m/s); where the flow regime remained laminar; This study could be repeated for higher ranges of velocities at the ranges of velocities ($V \geq 2$ m/s) at the future. As future work, we also perform experiments on the hexagonal channel contactor, and examine pressure drop, wall thickness effects, and hexagons side length. We will focus more on novel numerical methods and investigate using novel contactors shapes.

This is a preliminary study to shed light on the issue. Existing set of results are not covering a broad range, and we know that. However, most of the previous works are laboratory-scale experimental study and maneuver on the different aspects including fluid mechanic parts or technoeconomic. However, since types of studied barely done earlier, there is big differences on data reported by different authors, especially when it comes to cost estimation. Importance of these results are somehow can be shown on the cost dependence on pressure drop and air volume flow rate. At the future, if desorption phase is studied beside adsorption phase, this hexagonal geometry can be optimized for minimal consumption of electrical energy for unit of adsorbed CO₂.

REFERENCES

- Choi, S., Drese, J. H., Eisenberger, P. M., and Jones, C. W. (2011). Application of amine-tethered solid sorbents for direct CO₂ capture from the ambient air. *Environmental Science and Technology*, 45(6), 2420–2427.
- Cornejo, I., Nikrityuk, P., and Hayes, R. E. (2022). Heat and mass transfer inside of a monolith honeycomb: From channel to full size reactor scale. *Catalysis Today*, 383, 110–122.
- Deutschmann, O., Schwiedemoch, R., Maier, L. I., and Chatterjee, D. (2001). Natural gas conversion in monolithic catalysts: interaction of chemical reactions and transport phenomena. In *Studies in surface science and catalysis* (Vol. 136, pp. 251–258). Elsevier.
- Fu, D., and Davis, M. E. (2023). Toward the feasible direct air capture of carbon dioxide with molecular sieves by water management. *Cell Reports Physical Science*, 4(5).
- Hawthorn, R. D. (1974). Afterburner catalysts-effects of heat and mass transfer between gas and catalyst surface.
- Jiang, L., Liu, W., Wang, R. Q., Gonzalez-Diaz, A., Rojas-Michaga, M. F., Michailos, S., Pourkashanian, M., Zhang, X. J., and Font-Palma, C. (2023). Sorption direct air capture with CO₂ utilization. *Progress in Energy and Combustion Science*, 95, 101069.
- Klenov, O. P., Pokrovskaya, S. A., Chumakova, N. A., Pavlova, S. N., Sadykov, V. A., and Noskov, A. S. (2009). Effect of mass transfer on the reaction rate in a monolithic catalyst with porous walls. *Catalysis Today*, 144(3–4), 258–264.
- Kreutzer, M. T., Du, P., Heiszwolf, J. J., Kapteijn, F., and Moulijn, J. A. (2001). Mass transfer characteristics of three-phase monolith reactors. *Chemical Engineering Science*, 56(21–22), 6015–6023.
- Mazzotti, M., Baciocchi, R., Desmond, M. J., and Socolow, R. H. (2013). Direct air capture of CO₂ with chemicals: optimization of a two-loop hydroxide carbonate system using a countercurrent air-liquid contactor. *Climatic Change*, 118, 119–135.
- McQueen, N., Gomes, K. V., McCormick, C., Blumanthal, K., Pisciotta, M., and Wilcox, J. (2021). A review of direct air capture (DAC): scaling up commercial technologies and innovating for the future. *Progress in Energy*, 3(3), 32001.
- Raja, L. L., Kee, R. J., Deutschmann, O., Warnatz, J., and Schmidt, L. D. (2000). A critical evaluation of Navier–Stokes, boundary-layer, and plug-flow models of the flow and chemistry in a catalytic-combustion monolith. *Catalysis Today*, 59(1–2), 47–60.
- Rodríguez-Mosqueda, R., Bramer, E. A., and Brem, G. (2018). CO₂ capture from ambient air using hydrated Na₂CO₃ supported on activated carbon honeycombs with application to CO₂ enrichment in greenhouses. *Chemical Engineering Science*, 189, 114–122.
- Sanz-Pérez, E. S., Murdock, C. R., Didas, S. A., and Jones, C. W. (2016). Direct capture of CO₂ from ambient air. *Chemical Reviews*, 116(19), 11840–11876.
- Solomon, S., Plattner, G.-K., Knutti, R., and Friedlingstein, P. (2009). Irreversible climate change due to carbon dioxide emissions. *Proceedings of the National Academy of Sciences*, 106(6), 1704–1709.
- Thakkar, H., Eastman, S., Hajari, A., Rownaghi, A. A., Knox, J. C., and Rezaei, F. (2016). 3D-printed zeolite monoliths for CO₂ removal from enclosed environments. *ACS Applied Materials and Interfaces*, 8(41), 27753–27761.
- Tischer, S., and Deutschmann, O. (2005). Recent advances in numerical modeling of catalytic monolith reactors. *Catalysis Today*, 105(3–4), 407–413.
- Verougstraete, B., Martin-Calvo, A., der Perre, S., Baron, G., Finsy, V., and Denayer, J. F. M. (2020). A new honeycomb carbon monolith for CO₂ capture by rapid temperature swing adsorption using steam regeneration. *Chemical Engineering Journal*, 383, 123075.
- Wang, W., Wang, S., Ma, X., and Gong, J. (2011). Recent advances in catalytic hydrogenation of carbon dioxide. *Chemical Society Reviews*, 40(7), 3703–3727.
- Zhongming, Z., Linong, L., Xiaona, Y., Wangqiang, Z., Wei, L. (2021). *Global energy review 2021*. IEA: Paris, France.
- Nejadseifi, M., Kiani-Oshtorjani, M., Tynjälä, T., and Jalali, P. (2024). Permeability of partially to fully randomized arrays of square disks: A lattice Boltzmann approach. *Journal of Porous Media*, 27(3), 85–99.
- Nejadseifi, M., Tynjälä, T., Jalali, P., and Jere, Elfving. (under preparation). Adsorption of CO₂ by direct air capture in particle packed beds of sorbent: Direct simulation

approach. Under Preparation for Submission to Journal 'powder Technology'.

Jänchen, J., Herzog, T. H., Gleichmann, K., Unger, B., Brandt, A., Fischer, G., and Richter, H. (2015). Performance of an open thermal adsorption storage system with Linde type A zeolites: Beads versus honeycombs. *Microporous and Mesoporous Materials*, 207, 179–184.

Querejeta, N., Rubiera, F., and Pevida, C. (2022). Experimental study on the kinetics of CO₂ and H₂O adsorption on honeycomb carbon monoliths under cement flue gas conditions. *ACS Sustainable Chemistry and Engineering*, 10(6), 2107–2124.

Sakwa-Novak, M. A., Yoo, C.-J., Tan, S., Rashidi, F., and Jones, C. W. (2016). Poly (ethylenimine)-functionalized monolithic alumina honeycomb adsorbents for CO₂ capture from air. *ChemSusChem*, 9(14), 1859–1868.

Wajima, T., Munakata, K., Takeishi, T., Hara, K., Wada, K., Katekari, K., Inoue, K., Shinozaki, Y., Mochizuki, K., Tanaka, M., (2011). Adsorption characteristics of water vapor on honeycomb adsorbents. *Journal of Nuclear Materials*, 417(1–3), 1166–1169.

Choi, S., Drese, J. H., and Jones, C. W. (2009). Adsorbent materials for carbon dioxide capture from large anthropogenic point sources. *ChemSusChem: Chemistry and Sustainability Energy and Materials*, 2(9), 796–854.

Elfving, J., and Sainio, T. (2021). Kinetic approach to modelling CO₂ adsorption from humid air using amine-functionalized resin: Equilibrium isotherms and column dynamics. *Chemical Engineering Science*, 246, 116885.

Sanz-Pérez, E. S., Murdock, C. R., Didas, S. A., and Jones, C. W. (2016). Direct capture of CO₂ from ambient air. *Chemical Reviews*, 116(19), 11840–11876.